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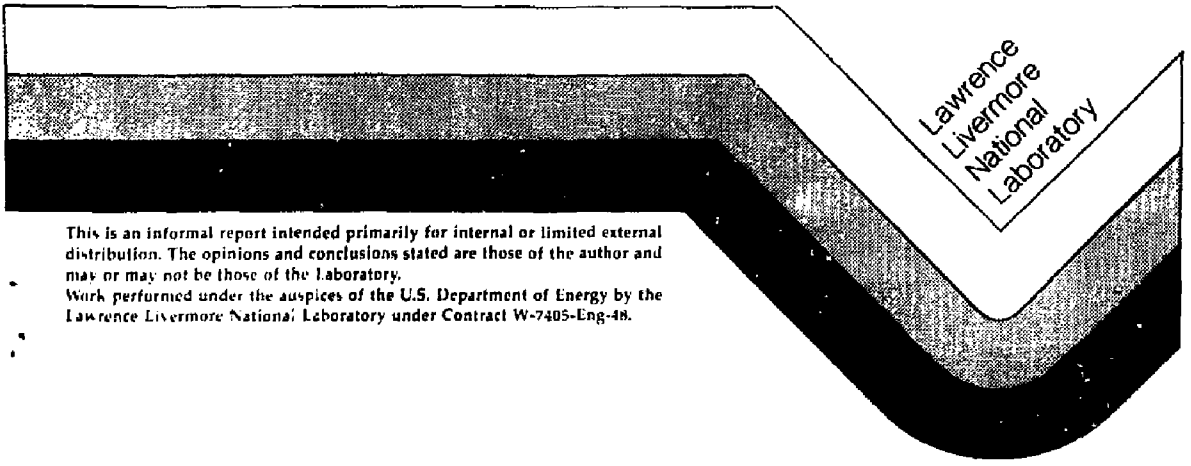
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UCID- 17530-89  
Revision 8

The Computational Physics Program  
of the National MFE Computer Center

Arthur A. Mirin

January 1989



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Work performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

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Printed in the United States of America  
Available from  
National Technical Information Service  
U.S. Department of Commerce  
5285 Port Royal Road  
Springfield, VA 22161

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## I. INTRODUCTION

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Since June 1974, the MFE Computer Center has been engaged in a significant computational physics effort. The principal objective of the Computational Physics Group is to develop advanced numerical models for the investigation of plasma phenomena and the simulation of present and future magnetic confinement devices. Another major objective of the group is to develop efficient algorithms and programming techniques for current and future generations of supercomputers. In addition, the group interacts with the systems programming staff to improve services; it fills the roles of internal critic and advisor by representing a user viewpoint. Moreover, many of the group's computer codes employ state-of-the-art algorithms that use and test the prototypical hardware and software features of the new machines; these codes have played a major role in perfecting the software supplied by NMFECC.

The group currently consists of six Ph.D. physicist/mathematicians - D.V. Anderson, G.D. Kerbel, A.E. Koniges, M.G. McCoy, A.A. Mirin and D.E. Shumaker. In addition, students (currently numbering 4) in the Department of Applied Science (U.C. Davis) are engaged in fusion research under the guidance of senior group members.

The computational physics group has been involved in several areas of fusion research. One main area is the application of Fokker-Planck/quasilinear codes to tokamaks. Another major area is the investigation of resistive magnetohydrodynamics in three dimensions, with applications to tokamaks and compact toroids. A third area is the investigation of kinetic instabilities using a 3-D particle code; this work is often coupled with the task of numerically generating equilibria which model experimental devices. Ways to apply statistical closure approximations to study tokamak-edge plasma turbulence have been under examination, with the hope of being able to explain anomalous transport. Also, we are collaborating in an international effort to evaluate fully three-dimensional linear stability of toroidal devices. In addition to these computational physics studies, the group has developed a number of linear systems solvers for general classes of physics problems and has been making a major effort at ascertaining how to efficiently utilize multiprocessor computers.

One of the principal objectives of the computational physics group is to provide support for experimental and theoretical work within the MFE community. At present, this support falls into the following areas:

|   |   |
|---|---|
| RF heating and current drive in tokamaks      | GA, ORNL, PPPL, MIT<br>AMPC, LLNL, Culham<br>Varenes (Quebec) |
| Fokker-Planck/transport analyses of tokamaks  | LLNL  |
| Tokamak equilibrium and stability             | U.C. Davis  |
| Compact torus transport/equilibrium/stability | LANL  |
| MHD evolution of Spheromak and FRC            | LANL, LLNL, Spectra   |

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Turbulence models in plasma physics

PPPL, LLNL, UCSD

Direct matrix solvers/3-D equilibrium  
and stability calculations

Ecole Polytechnique  
Federale de Lausanne

A summary of our program follows.

## II. COMPUTATIONAL STUDIES

### A. EQUILIBRIA AND STABILITY

#### 1. TIME INDEPENDENT MODELS

In simple 1-D configurations the calculation of plasma equilibrium profiles is rather trivial. For more realistic two and three dimensional plasmas, the determination of the equilibrium magnetic fields and the plasma pressure is a complicated nonlinear problem involving the solution of elliptic partial differential equations. One of the goals of this work is to obtain configurations like those seen in experiments; accordingly some of our calculations use boundaries and external coil sets which accurately represent the devices under study. A secondary goal is to compute equilibria of sufficient accuracy so that the results can be used by stability codes with some confidence. In this connection high order finite element or finite difference representations have been used. These equilibria are also used to explore single particle effects in equilibrium magnetic fields.

Most of our codes solve Ampere's law given some nonlinear dependence of the currents on the fields. Other codes use a dynamic evolutionary approach with artificial damping to obtain steady flow equilibria. Still others merely numerically evaluate known analytical equilibrium profiles. Several of these codes are briefly described in Table 1.

Our research has been in the following areas:

•A code was developed to solve the 2D MHD equilibrium problem for compact toroids. The algorithm is applicable to elongated plasmas. Finite elements are used to solve the Grad-Shafranov equation. The region in which the equilibrium is computed may contain a separatrix, and plasma may be present both inside and outside of the separatrix. The equilibrium is determined from adiabatic quantities, magnetic fluxes and entropy; hence, the solver is suitable for insertion in a transport code. This code has been documented and made available to the fusion community.

•A 2D kinetic equilibrium code for compact toroids has recently been developed. The distribution functions depend on the Hamiltonian and the canonical angular momentum; the electrostatic potential is obtained from quasineutrality. The code can also compute zero-electron-temperature equilibria; in this case the electrostatic potential is an input quantity.

•Tandem mirror equilibrium calculations have been undertaken in 3D, with the goal of making the simulations as realistic as possible. A multispecies plasma is modeled in a multi-region configuration to account for the various types of trapped and passing components known to exist in these devices. Ambipolar effects are included. High beta and finite curvature effects are modeled without making low beta or long-thin approximations. A finite element representation is used on a rectangular grid. The effect of sheath formation has been shown to be in agreement with other theory and experiments. Some species, such as sloshing ions, are poorly represented by adhoc pressure functions, so these are being supplemented by models using correct moments of microscopic distribution functions. Comparison with models using the paraxial approximation have been carried out. It appears that the long-thin approximation is not valid for most realistic mirror configurations.

•A code which computes the vacuum magnetic field inside a toroidal vessel of arbitrary cross-section was developed and applied to HELIAC. General curvilinear coordinates conforming to the shape of the vessel are used. The magnetic scalar potential is expanded as a double Fourier series in the poloidal and toroidal angles. The resulting magnetic fields have been evaluated for their minimum-average-B and shear stability properties using the field line tracing code TUBE. The aim has been to find optimum vessel configurations by calculating the resulting surface currents and later discretizing these skin currents with closed current loops.

•The three dimensional stability of three dimensional toroidal ideal MHD equilibria is being addressed in a new code, TERPSICHORE, being built as a collaborative effort between ourselves and European colleagues in Germany and Switzerland. Rather general stellarator and tokamak configurations are representable in this code which uses finite Fourier series to parameterize each closed toroidal flux tube. Assuming the validity of the given equilibrium configurations, the code can be used to determine stability limits, second stability regions, and optimal coil specifications.

Our time-independent equilibria and stability publications are summarized in Appendix A1.

## 2. TIME DEPENDENT MAGNETOHYDRODYNAMICS

A principal technique for determining macroscopic plasma behavior is through the solution of the time dependent MHD equations. Of particular interest is the nonlinear evolution and saturation of fluid instabilities. Accurate simulation of such phenomena requires the solution of the full set of MHD equations, which comprises a coupled system of eight nonlinear partial differential equations. This is a formidable task for any computer system. In order to make these computations tractable, approximations have often been made, including reduction in

dimensionality, linearization, restriction to a particular geometry and the assumptions of infinite conductivity and/or low "beta" ("beta" is the ratio of plasma pressure to magnetic pressure). The infinite conductivity assumption (called ideal MHD) greatly simplifies the numerics, since the MHD equations are then hyperbolic rather than parabolic. Moreover, resistive MHD instabilities tend to grow more slowly than ideal MHD instabilities, thereby requiring longer running times. The low beta assumption allows an ordering in which the problem is reduced to the solution of two scalar equations.

At the MFECC, the emphasis has been on constructing resistive MHD codes which are applicable to all plasmas. Both linear and nonlinear codes have been written which solve the full set of resistive, "finite-beta" MHD equations in two and three dimensions (see Table 2). Moreover, most of these codes use an implicit time discretization, so that there is no restrictive non-physical upper bound on the size of the timestep.

Our MHD research has been in the following areas:

- Linear studies of resistive interchange modes in the reversed field pinch were carried out using a two-fluid code. These simulations included Hall terms and tensor thermal conductivities and viscosities. It was shown that Hall and electron thermal conduction effects together (but neither alone) would provide stabilization.

- A 3D nonlinear, resistive, initial-value, compressible code has been used to model a cylindrical reversed field pinch. In one application, this code, along with four other 3D codes (developed at other institutions), has simulated an identical problem to try to ascertain the effects of compressibility in RFP dynamics. The study showed that compressibility could be instrumental in determining field reversal maintenance.

- Our nonlinear 3D code has been applied to the behavior of resistive modes in a spheromak. Whether or not a general equilibrium relaxes to a force free state, and if it does, how long it takes and how the relaxation is affected by MHD modes, has been under investigation. The effects of Hall terms are included.

- The nonlinear 3D code described above has been modified to include implicit differencing. For the purposes of economizing computer time, a multitasked semi-implicit technique has been implemented. Hall terms are also treated semi-implicitly. Implicit simulations of the spheromak have been carried out, with a factor of 30 savings in computer time. Studies have recently been under way to analyze the effectiveness of the semi-implicit method for simulations with Hall terms. Toward this aim, calculations relevant to spheromak, FRC, and RFP scenarios have been carried out.

•Investigations have begun into the possibility of fueling a tokamak reactor such as ITER through the injection of compact toroids (CT's). It is believed that such a technique may be necessary since conventional fueling methods may not be adequate for deep penetration. One of the critical issues with such a scheme is magnetic reconnection, for it plays a major role in determining where and when the fuel is deposited. Our present calculations start with a CT being placed at rest in a uniform magnetic field modified to exclude the CT. Preliminary results show the CT tilting in roughly an Alfvén time as its internal structure decomposes.

•A study of the stability of long, thin theta-pinch equilibria to the  $n = 1$  tilt mode was undertaken. Earlier numerical work predicting a fast growing tilt instability was in contradiction to the long quiescent times of the experiments. The hypothesis that the computations were based on incorrect models of the theta pinch equilibrium is now refuted. Usage of a resistive MHD stability code has shown that stretching of the closed elliptical flux surfaces (making them more racetrack as in the experiments) is destabilizing. The stability of these devices to this mode is due to effects beyond the MHD model. In particular, kinetic effects must be taken into consideration.

Our time-dependent MHD publications are summarized in Appendix A2.

## B. PLASMA TRANSPORT

Transport codes are used to evaluate macroscopic plasma parameters (e.g. density, temperature) on a timescale comparable to the lifetime of the plasma. They differ from other fluid codes in that the fast timescale physics is integrated out of the problem.

At the MFEC, transport codes have been applied to tokamaks, compact toroids and tandem mirrors. A list of our transport codes and their applications appears in Table 3.

Over the past years we have made a great deal of progress in the following areas:

- Fokker-Planck/transport studies of tokamaks
- Anomalous electron transport in tokamaks
- Transport in compact toroids
- Radial transport in tandem mirrors

We have also been looking into plasma turbulence as an explanation for anomalous transport (see Section F).

A brief summary follows.

•Fokker-Planck/Transport Studies of Neutral Beam-Heated Tokamaks

Neutral beam-heated tokamaks are characterized by the presence of one or more energetic ion species which are quite non-Maxwellian along with a warm Maxwellian bulk plasma. For scenarios in which there is a large energetic ion population, it is very important to represent these energetic species by means of velocity space distribution functions and to follow their evolution in time by integrating the Fokker-Planck equations. It is essential to utilize the full nonlinear Fokker-Planck operator to assure that the slowing down and scattering of these energetic species is computed accurately and realistically.

Our Fokker-Planck/transport code (FPT), in addition to solving radial transport equations for the bulk plasma densities and temperatures, solves nonlinear Fokker-Planck equations in 2D velocity space for the energetic ion distribution functions. The FPT code is unique in that it is the only tokamak transport code which does not either linearize the Fokker-Planck operator or ignore it altogether. Also, neutral beam deposition and neutral transport are computed using appended Monte Carlo codes developed at Princeton.

During the last decade FPT has been applied to a number of experiments. Most recently it has been used to model TFTR and ITER. The TFTR simulations have concentrated on ascertaining the beam-beam, beam-target and thermonuclear fusion rates; excellent agreement with the "supershot" results is obtained. The ITER simulations have concentrated on evaluating the effectiveness of neutral beam current drive; efficiencies comparable to those of rf schemes are obtained.

•Anomalous Electron Transport in Tokamaks

Over the years, there has been considerable interest in the effects of anomalous electron transport due in part to magnetic surface destruction. Since this heat loss represents a major problem in toroidal confinement, there has been a need for a program which would simulate this loss and allow for credible estimates of the effects of electron transport on lower hybrid heating, D.C. conductivity and soft x-ray spectra.

The computer program (LDL) which has consequently been developed is 2-D and has as independent variables velocity magnitude and radial position. It combines a velocity and radially dependent heat source and a 1-D Fokker-Planck treatment of electron collisions with a loss operator simulating diffusion in velocity-radius. This program has been applied to the Doublet experiments at GA Technologies, Inc.

•Transport in Compact Toroids

The compact torus experiments (field reversed theta pinch and spheromaks) differ from the tokamak in that the plasma extends to the axis of rotational symmetry. Interest in the compact torus is due to the fact that it is likely to attain high beta and the fact that there is an engineering advantage of not having any structure through the center of the torus.

A transport code, CTT, has been written to describe the evolution of the plasma and magnetic field in a compact torus. This code differs from the tokamak transport codes in that the plasma extends to the axis of rotational symmetry and the 2-D equilibrium calculation contains a separatrix. The system evolves by alternating between the solution of four 1-D transport equations and the calculation of a 2-D equilibrium. The independent variable is the poloidal magnetic flux. Classical diffusion, Pfirsch-Schluter diffusion, radiation, Joule heating, lower hybrid drift diffusion and open field line loss are modeled.

The code has been used to model the FRX and the CSS experiments. In the former case good agreement with the experiment is obtained provided the collision frequencies are appropriately enhanced; discrepancies along the open field lines, however, point to the need for 2D modeling in that region.

•Radial Transport in Tandem Mirrors

A tandem mirror machine consists of a long, solenoidal cell with minimum-B mirrors (plugs) at either end which act to electrostatically confine the central cell ions. The rate at which charged particles and heat diffuse in radius is of crucial importance. Of special significance is the expected enhanced transport of ions due to resonance between their azimuthal drift and axial bounce motions, which results from the presence of a non-axisymmetric magnetic field in the transition regions between the end plugs and the solenoid. A radial transport code, TMT, was written in order to investigate this and other related phenomena. This multispecies code computes radial profiles of densities and temperatures in both the central solenoid and the end plugs along with a self-consistent electric field. Classical and neoclassical effects on transport are taken into account. This code has been used to study the Tandem Mirror Experiment and to help design larger tandem mirror devices.

Our transport publications are summarized in Appendix B.

C. FOKKER-PLANCK

The Fokker-Planck equation is needed to treat plasmas in which the charged particle velocity space distribution functions are non-Maxwellian. In a magnetic mirror device, charged

particles will tend to leak out the ends of the device, resulting in a "loss cone" in velocity space. In devices where there is neutral beam injection, rf heating or a large d.c. electric field, the ion distribution functions will be characterized by an energetic component (in addition to the Maxwellian background). These are situations which require the use of Fokker-Planck codes.

The MFECC has led the nation in the development and implementation of multispecies Fokker-Planck codes employing the complete nonlinear two-dimensional Fokker-Planck operator. Since our codes have been generalized to deal with toroidal and open-ended configurations, many physical effects have been incorporated in them and a variety of physical problems have been studied. A summary of our Fokker-Planck codes appears in Table 4.

Progress has been made in the following areas:

- We developed a user-oriented package, FPPAC, which computes the coefficients of the uniform-field nonlinear 2D velocity-space Fokker-Planck collision operator and time-integrates the corresponding finite difference equations. The user may specify additional physics terms and rather arbitrary boundary conditions. FPPAC has been made available to the MFE community.

- A nonlinear multispecies Fokker-Planck code (CQL) which bounce-averages the differential operators of Coulomb collisions, quasilinear resonant diffusion induced by wave-particle interaction and an Ohmic electric field has been developed. A zero banana width is assumed. CQL is designed primarily to simulate toroidal devices, although it can be utilized for mirror applications. The relativistic collisional coefficients incorporate an arbitrary number of terms in the Legendre expansion of the distribution functions. The rf operator incorporates mass shift, spectral and collisional resonance broadening and models waves at the electron cyclotron, ion cyclotron and lower hybrid frequencies. CQL has recently been put in package form and released to the MFE community.

- To obtain a global view of tokamak operation, the two dimensional  $(v, \theta)$  code CQL described above has incorporated a three dimensional module, together called CQL3D, which allows the calculation to proceed at several radial mesh points simultaneously. Due to the bounce averaging, the resulting picture is, in most cases, actually four dimensional, if one considers the poloidal perspective. The 3D version is well suited to implementation in a multitasking environment since the distribution functions at the various radial meshpoints are advanced independently. A wave damping calculation to compute electric fields and other relevant wave parameters as a function of position (radial and poloidal) provides linkage between the radial meshpoints. CQL3D is intended for use primarily on the Cray-2.

•A number of studies have been undertaken with the CQL family. In collaboration with G.A., fusion reactivity enhancement by ICRF has been examined; at high Q the enhancement factor ranges from 1.3 to 2.0. A more recent application of the code examines the relative merits of inside vs. outside launch schemes for ECH current drive, with particular attention to relativistic effects. The CQL study advises an outside launch, which is contrary to what is currently being done in D3D. Present efforts include (1) a coupling of CQL3D to the GA transport code ONETWO and the Princeton/Oak Ridge neutral beam code NFREYA; this will allow global simulation of tokamak performance and the determination of neutral beam current drive efficiency in devices such as ITER; this has included generalizing CQL to accept noncircular cross-sections; (2) coordination between the full wave propagation calculations for ICRH and ray optics calculations for ECRH and the consequent quasilinear development of the underlying distributions; (3) the use of CQL to evaluate linear growth rates and saturated wave amplitudes for beam-driven instabilities; and (4) relaxation of the zero-banana-width restriction to allow the calculation of non-Maxwellian corrections to neoclassical transport coefficients (applicable to alpha, neutral beam, and rf heated plasmas).

•Tandem Mirror Applications

A study of electrostatically trapped electrons in a tandem mirror thermal barrier has recently been completed. This has required solving Fokker-Planck equations for trapped electrons in the presence of passing electrons and under the influence of electron cyclotron resonant heating.

Calculations of fusion performance in D-D tandem mirrors have also been completed. Fokker-Planck equations for deuterons and the four reaction products have been solved. Radiation losses, recycling and drift pumping for ash removal have been included. Some p-based calculations have also been carried out.

A 2D nonlinear multispecies code has been used to assess trapping rates of passing ions in tandem mirror end cells. A scaling law valid over a wide range of mirror ratio, trapping parameter and potential-to-temperature ratio has been developed.

Our Fokker-Planck publications are summarized in Appendix C.

D. PARTICLE AND VLASOV MODELS

•Three-Dimensional Particle Code

A 3-D quasi-neutral hybrid particle-in-cell code which models ions as particles and electrons as a massless, zero-temperature fluid has been developed for the Cray-2. Unlike earlier particle codes that required disk memory and scalar

interpolation, tedious coding of buffered disk memory and the corresponding waste of CPU time have been eliminated and new algorithms which allow every phase of the calculation of be vectorized and multitasked have been developed. The interpolation between the grid and the particles has been coded in terms of indirect indices and executes in vector mode via the hardware gather and scatter instructions. An optimized particle sorting scheme consistent with vectorization has been developed. The fields are computed on a cylindrical grid in such a way as to guarantee a solenoidal magnetic field. The vacuum region is modeled as a resistive medium. Studies of Field Reversed Configurations have been undertaken. As a benchmark, the rotational instability of the rigid rotor was modeled and found to agree with a 2D particle code; for this purpose a special treatment of the low density regions had to be incorporated. The code has recently been applied to a study of the nonlinear evolution of the tilt mode instability in a FRC. It is shown that in the large gyroradius limit kinetic effects stabilize the mode. The growth rates are in fair agreement with linear calculations using a kinetic model. Simulations into the nonlinear regime are being undertaken.

•We have written a code called ORB which solves the equations of motion associated with Littlejohn's guiding center Hamiltonian theory for tokamak geometry. Included are several model wave field excitations for studying wave-particle interaction in three dimensions. The code includes a facility for representing the orbit in terms of its (slowly varying) first order instantaneous constants of motion. To do this, the current state of motion is interpreted through the zeroth order Hamiltonian to get the corresponding adiabatic invariants. ORB is used in conjunction with our bounce-averaged Fokker-Planck code CQL3D and is an important ingredient of our transport effort.

•A self-consistent guiding center particle model coupled with a fluid equilibrium code was used to study ion beam motion in a toroidal geometry. Applications include the study of collisionless beam behavior in the case of strong counterstreaming beams and the steady state modeling of a CIT reactor, in which beam currents and energy reinjection rates are computed.

•A single particle orbit following code was used to make detailed studies of the confinement properties of equilibrium fields in two and three dimensions. Studies of adiabaticity as well as resonant orbital effects were made. Experimentalists used the code to design ion probe diagnostics.

•A one-dimensional Vlasov finite difference code for ions and electrons was written to study the formation of a plasma sheath and to compute steady state distribution functions along with a plasma potential.

Publications in this area are listed in Appendix D.

## E. EFFICIENT NUMERICAL ALGORITHMS AND PROGRAMMING TECHNIQUES

### •Solution of Sparse Implicit Systems

A general study of Preconditioned Conjugate Gradient Methods for solving sparse linear systems is being carried out. This technique has been shown to be considerably faster than other traditional linear solvers such as SOR and ADI. Solvers applicable to both scalar and vector 2D and 3D operators have been written and made available to the MFE community. These solvers incorporate (as an option) the biconjugate gradient (BCG) method. BCG tends to converge faster than ordinary CG and is more amenable to multitasking. A multitasked form of the BCG solvers is available. The use of vectorized indirect indexing has made it possible to produce packages applicable to various mesh stencils and sparsity patterns with a minimum of effort. In this connection a fully implicit Maxwell's equation solver in which the various field components are closely coupled has been built and tested. Our sparse matrix solvers, which are listed in Table 5, have been/are being published to provide adequate documentation and allow easy access by other users.

Performance measurements of our solvers for coupled PDE's shows a degradation in computing speed by a factor of four from what could be obtained using assembly language. Even with assembly code, there is still considerable room for improvement both from the standpoints of parallelization and convergence rates. Based on some recent successes on related problems, we are investigating the properties of preconditioners based upon incomplete matrix inversion.

### •Solution of Block-Banded Systems

In some applications the structure of the resulting matrix system is block tridiagonal with dense blocks. This kind of structure arises from the use of spectral representations in one or more of the coordinate directions. We have developed a new code, PAMS, that solves this type of system. PAMS has been designed to exploit the three forms of parallelism available on the Cray-2 - multitasking, vectorization and functional unit overlap. Speeds in excess of 1.2 Gflops have been measured, thus making PAMS one of the fastest codes available on the Cray-2. PAMS has also been used as a benchmark for vector supercomputers. It has been tested on the Cray-X/MP, Cray-2, Fujitsu VP-200, NEC SX-2, CDC-205, and the ETA-10 Piper. It has been extended to solve more general block multidagonal systems and is part of an eigensolver in a 3-D stability code.

### •Multitasking

The CRAY-XMP and CRAY-2 computers possess more than one CPU and hence have the capability of parallel computation. Computer codes that require large fractions of the central memory or that need fast real time performance can benefit if they are written such that parallel computation is feasible. This mode of

calculation is referred to as multitasking in the CRAY environment. The computational physics group is investigating the efficient utilization of the CRAY-2 in this direction. Some of our multitasking applications have been discussed in the above section on sparse matrix solvers. A brief summary of our other multitasking applications follows.

•The VEPEC code, which computes 3D tandem mirror plasma equilibria (see Table 1), has been used as a test bed for studying multitasking in the CTSS environment. The idea here has been to ascertain the extent to which existing codes can be converted to multitasking without too much rewriting. The efficient multitasking of a vectorized 3D ADI solver appropriate for certain nonlinear problems has been demonstrated. This shows the perhaps unexpected value of multitasking even for tightly coupled implicit systems. Another important issue is the cost of the overhead required to implement multitasking--this is closely related to the granularity of the tasks. A further objective has been to provide feedback as to the design of the operating system, where in fact VEPEC experience led to a new system scheduler that gives greatly improved multitasking performance.

•Our multitasked simulation code (SIMU) uses the concept of ensemble averaging to solve a prototypical three-wave interaction problem. The use of ensemble averaging, as opposed to time-averaging, turns the problem into an ideal candidate for multitasking. Since realizations of the dynamical equation can be grouped into arbitrary-sized packets, the multitasking nature of the code can be adapted for machines with arbitrary numbers of processors - from four to four thousand. In order to run SIMU and guarantee reproducible results independent of the multitasking, we require a means of producing strings of random numbers for each process. This problem is very important in all Monte-Carlo calculations run on multiprocessor computers. We have devised a method for producing independent strings based on hopping through a random number sequence at large intervals and picking up a seed for each process. This method is particularly useful for our application and shows promise for use in general Monte Carlo codes.

•Another important issue is the degree of multiprocessing efficiency one should expect to get under CTSS, which is an intense time-sharing environment. In this regard we have used our 3-D MHD code TEMCO to study multitasking performance as a function of task size and code field length. This has led to a theoretical model designed to predict the multiprocessing performance under CTSS. This model shows, for example, that (assuming the time to get an additional processor is 6 ms) a multitasking job must have a field length of at least 10 Mwds if an overlap factor of 3.5 is to be attained. We have found in general that the CTSS scheduler allows good overlap provided the code is large and the task string (i.e. the set

of tasks which are available to run consecutively on a processor) is of medium-to-large granularity.

•The previously mentioned TERPSICHORE code is an example of a new code developed from scratch with multitasking designed into it. We used the PAMS algorithm as a basic component of the code's eigenvalue solver. Moreover, it has been found that the large arrays of flux tube integrals required to determine the matrix operator coefficients may be rapidly computed from matrix-matrix products that are trivially multitaskable. A construct testing this idea has run at speeds of up to 1.73 Gflops on our new static memory Cray-2. This is presently being installed in the TERPSICHORE code.

Our multitasking codes are summarized in Table 6.

Publications in efficient numerical algorithms and programming techniques are summarized in Appendix E.

#### F. PLASMA TURBULENCE AND ANOMALOUS TRANSPORT

Strong turbulence is a leading candidate to explain anomalous transport in tokamak plasmas. Only theories which incorporate fully nonlinear effects of strong turbulence have the potential for predicting the large anomalous transport coefficients believed present in modern devices. The primary means of studying strong turbulence include analytic predictions, turbulence closure models, and direct simulation. The following are areas in which we are active.

##### •Ensemble Averaging

The most fundamental way to simulate turbulent phenomena is to time-advance the nonlinear equations and average over a Gaussian ensemble of initial conditions. Although this is not a practical means for describing complex systems, applying it to simple systems provides considerable insight into the relevant statistical dynamics. We have written a multitasked 3-wave simulation code for the purpose of studying plasma-type systems which contain inherent driving and damping. Such systems are fundamentally different from the viscous Navier-Stokes equations, which require external forcing to achieve steady states. We have used this code to study the drift wave system. The primary results show that certain assumptions such as the decay of correlation functions and the applicability of a fluctuation-dissipation relation can be used in some (but not all) situations.

##### •Two-Point Closures

In principle, turbulence closures can provide a theoretical understanding as well as predictions of turbulent flow properties. We are developing a program aimed at investigating the feasibility of two-point closures for complex calculations. In particular, we are considering new algorithms to accelerate

numerical computation of the class of closures typified by Kraichnen's Direct Interaction Approximation (DIA). We are developing a closure theory which is both applicable to plasma turbulence and amenable to numerical solution. Approximations based on the physics of the turbulent steady state are potentially useful for simplifying the numerical computation. In particular, we have used numerical simulation to show that the fluctuation-dissipation relation is a reasonable approximation for a damped/driven system in steady state. Our current scheme incorporates this approximation, and in doing so, eliminates a costly integration present in full DIA calculations. Finally, we are investigating a procedure based on Pade approximates which simplifies the problem further. Additionally, this method eliminates the need for the introduction of ad hoc parameters (usually based on estimates of the eddy viscosity) in models of the Markovian type.

•Applications to Multifield Systems

Analytic investigation of tokamak turbulence evolution equations has implied that even a minimal dynamical description of drift wave turbulence requires two-field evolution equations for the density and potential functions. We are planning to study the equilibrium statistical mechanics of the two-field Hasegawa-Wakatani model of drift wave turbulence. Additionally, we will examine the importance of the cross-correlation spectrum which has been traditionally neglected in Markovian closure calculations for fluid dynamic applications. We seek to quantify notions of a nonlinear transfer rate in terms of entropy production, and to verify analytic estimates of relaxation spectra.

G. OTHER AREAS

We have undertaken some projects in other areas, as follows:

•Convergent Neutral Beams

A study was made involving the creation of a very dense plasma by injecting convergent neutral beams into spherical or cylindrical chambers. Calculations of particle distribution functions, densities, ionization rate parameters and ionization probabilities were carried out for both geometries.

Publications in these areas are summarized in Appendix G. Miscellaneous publications are listed in Appendix H.

TABLE 1. MFECC TIME INDEPENDENT CODES

| CODE          | CONTACT         | CHARACTERISTICS AND APPLICATIONS  |
|---------------|-----------------|---|
| CYLEQ         | D.V. ANDERSON   | 2D (R,Z), Bicubic Splines, Finite Element, Tensor Pressure; Tandem Mirrors, Compact Toroids                                       |
| VEPEC         | D.V. ANDERSON   | 3D (X,Y,Z), Tricubic Splines, Finite Element, Vector Potential, Tensor Pressure, Ambipolar Effects, Vlasov Species Tandem Mirrors |
| ABCXYZ, TPSIC | D.V. ANDERSON   | Auxiliary codes for VEPEC   |
| HILLSV        | D.V. ANDERSON   | Auxiliary code for CYLEQ  |
| EIV           | D.E. SHUMAKER   | 2D, Flux Coordinates, Finite Elements, Open and Closed Field Lines; Compact Toroids   |
| EQV           | D.E. SHUMAKER   | 2D, Kinetic Equilibria, Flux Coordinates, Finite Elements, Open and Closed Field Lines; Compact Toroids                           |
| VAFIS         | A.I. SHESTAKOV* | 3D, Double Fourier Series, General Coordinates; Stellarators, HELIAC  |
| TUBE          | A.A. MIRIN      | Field Line Tracing Code; General Magnetic Fields  |
| STABCRIT      | D.V. ANDERSON   | 2D (R,Z) Ballooning Modes, Energy Principle   |
| TERPSICHORE   | D.V. ANDERSON   | 3D Displacements of 3D Toroidal Equilibria; Tokamaks, Stellarators  |

\*Currently in CP-Division (LLNL)

TABLE 2. MFECC TIME DEPENDENT MHD CODES

| CODE      | CONTACT         | CHARACTERISTICS AND APPLICATIONS   |
|-----------|-----------------|--|
| TEMCO     | A.A. MIRIN      | 3D (R, $\phi$ ,Z), Nonlinear, Semi-Implicit, Resistive, Fourier Expansion in $\phi$ , Viscous, Hall terms; Compact Toroids, RFP        |
| RIPPLE VI | A.I. SHESTAKOV* | 2D (R,Z), Linear, Nonaxisymmetric Perturbations, Implicit, Resistive; Compact Toroids  |
| ALIMO     | A.I. SHESTAKOV* | 2D (R,Z), Linear, Axisymmetric Perturbations, Implicit, Resistive; Compact Toroids   |
| RIPPLE V  | A.I. SHESTAKOV* | 1D (y), Linear, Implicit, Equilibrium Flow   |
| RIPPLE IV | A.I. SHESTAKOV* | 1D (r), Linear, Implicit, Resistive; Tokamaks, RFP   |
| ODRIC     | A.A. MIRIN      | 1D (r), Linear, Implicit, Resistive, Compressible, Tensor Viscosity, Tensor Thermal Conductivity, Hall terms, Two-Fluid; Tokamaks, RFP |

\*Currently in CP-Division (LLNL)

TABLE 3. MFECG TRANSPORT CODES

| CODE      | CONTACT       | CHARACTERISTICS AND APPLICATIONS   |
|-----------|---------------|--|
| TMT       | A.A. MIRIN    | 1D (R); Tandem Mirrors   |
| FPT       | A.A. MIRIN    | Combined Fokker-Planck/Transport,<br>1D (R) plus 2D (V, $\theta$ ); Tokamaks |
| CTT       | D.E. SHUMAKER | 1D (Poloidal Flux)/2D Equilibrium; Compact<br>Toroids                        |
| TRANSPORT | A.A. MIRIN    | 1D (R); Tokamaks   |
| LDL       | M.G. McCOY    | 2D (R,V); Electron Transport;<br>Tokamaks                                    |

TABLE 4. MFECC FOKKER-PLANCK CODES

| CODE      | CONTACT                   | CHARACTERISTICS AND APPLICATIONS  |
|-----------|---------------------------|---|
| HYBRID II | A.A. MIRIN                | 2D (V, $\theta$ ), Nonlinear, Multispecies Ions; Mirrors and Tokamaks   |
| TDMFP     | A.A. MIRIN                | 2D (V, $\theta$ ), Nonlinear, Multispecies Ions and Electrons; Mirrors  |
| TDMSZ     | A.A. MIRIN                | 3D (V, $\theta$ ,Z), Nonlinear, Multispecies Ions and Electrons   |
| FPFAC     | M.G. McCOY<br>A.A. MIRIN  | 2D (V, $\theta$ ), Nonlinear, Multispecies Ions; General Package  |
| ISOTIONS  | A.A. MIRIN                | 1D (V), Nonlinear, Multispecies Ions and Electrons; Mirrors and Tokamaks  |
| CQL       | M.G. McCOY<br>G.D. KERBEL | 2D (V, $\theta$ ), Nonlinear, Bounce Average, Multispecies Ions, Quasilinear rf. Relativistic, Noncircular Cross-sections; Tokamaks                       |
| CQL3D     | M.G. McCOY                | 3D (r,V, $\theta$ ), Nonlinear, Bounce Average, Multispecies Ions and Electrons, RF with Wave Damping, Relativistic, Noncircular Cross-sections; Tokamaks |
| RFT       | G.D. KERBEL               | Trajectory Integral Propagator and Data Base Generator for CQL  |
| ORB       | G.D. KERBEL               | Guiding Center Hamiltonian Orbit Code used in Conjunction with CQL  |

TABLE 5. MFECC ITERATIVE MATRIX SOLVERS

| CODE       | CONTACT       | PURPOSE               |
|------------|---------------|-----------------------|
| ICCG2      | D.V. ANDERSON | 2D Symmetric, Scalar  |
| ICCG3      | D.V. ANDERSON | 3D Symmetric, Scalar  |
| ILUCG2     | D.V. ANDERSON | 2D Asymmetric, Scalar |
| ILUCG3     | D.V. ANDERSON | 3D Asymmetric, Scalar |
| ILUBCG2    | A.E. KONIGES  | 2D Asymmetric, Scalar |
| CPDES2     | D.V. ANDERSON | 2D Asymmetric, Vector |
| CPDES3     | D.V. ANDERSON | 3D Asymmetric, Vector |
| MTBCG2     | A.E. KONIGES  | 2D Asymmetric, Scalar |
| MTCS2      | A.E. KONIGES  | 2D Asymmetric, Vector |
| MTCS3      | A.E. KONIGES  | 3D Asymmetric, Vector |
| ILUBCG2-11 | A.E. KONIGES  | 2D 11-Banded          |

TABLE 6. MFECC MULTITASKING CODES

| CODE                     | CONTACT       | PURPOSE                  |
|--------------------------|---------------|--------------------------|
| VEPEC                    | D.V. ANDERSON | Plasma Equilibria        |
| MTBCG2<br>MTCS2<br>MTCS3 | A.E. KONIGES  | Iterative Matrix Solvers |
| QN3D<br>HQC              | D.E. SHUMAKER | Particle Code            |
| SIMU                     | A.E. KONIGES  | Turbulence               |
| PAMS                     | D.V. ANDERSON | Direct Matrix Solver     |
| TEMCO                    | A.A. MIRIN    | MHD Evolution/Stability  |
| TERPSICHORE              | D.V. ANDERSON | MHD Stability            |

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